

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061824\
 Data File : VU059330.D
 Acq On : 18 Jun 2024 22:38
 Operator : MD/SY
 Sample : P2873-19ME
 Misc : 3.10g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 38 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0SK8ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
 Title : VOC Analysis

Signal : TIC: VU059330.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.592	86	94	122	rVB	51114	84980	12.07%	1.402%
2	1.821	137	165	168	rBV4	40715	145909	20.73%	2.408%
3	2.370	329	336	342	rBV6	1562	2073	0.29%	0.034%
4	2.538	377	388	404	rVB	130176	211207	30.00%	3.485%
5	2.724	443	446	449	rVB2	356	232	0.03%	0.004%
6	2.769	454	460	465	rVB4	567	827	0.12%	0.014%
7	2.798	466	469	473	rVB3	279	201	0.03%	0.003%
8	2.936	508	512	514	rBV2	330	228	0.03%	0.004%
9	3.026	531	540	550	rBV3	4371	8022	1.14%	0.132%
10	3.171	577	585	594	rBV2	730	1621	0.23%	0.027%
11	3.325	630	633	637	rVB	258	211	0.03%	0.003%
12	3.451	668	672	680	rVB	355	406	0.06%	0.007%
13	3.496	682	686	690	rBV	308	299	0.04%	0.005%
14	3.682	739	744	747	rVB3	359	303	0.04%	0.005%
15	3.766	765	770	777	rVB2	273	420	0.06%	0.007%
16	3.843	789	794	796	rBV2	305	261	0.04%	0.004%
17	3.888	805	808	811	rVB	287	194	0.03%	0.003%
18	4.001	839	843	849	rVB	246	217	0.03%	0.004%
19	4.248	916	920	923	rBV2	243	210	0.03%	0.003%
20	4.335	943	947	951	rBV2	271	280	0.04%	0.005%
21	4.357	951	954	958	rVV2	298	257	0.04%	0.004%
22	4.428	972	976	978	rBV2	297	259	0.04%	0.004%
23	4.621	1025	1036	1074	rBV	64260	185967	26.42%	3.069%
24	4.936	1128	1134	1137	rBV2	221	300	0.04%	0.005%
25	5.052	1152	1170	1194	rBV	127246	283634	40.29%	4.680%
26	5.370	1264	1269	1274	rBV2	192	259	0.04%	0.004%
27	5.557	1324	1327	1330	rBV2	265	207	0.03%	0.003%
28	5.711	1356	1375	1398	rBV2	263922	703992	100.00%	11.616%
29	5.859	1417	1421	1425	rVB4	336	342	0.05%	0.006%
30	5.904	1432	1435	1438	rVB2	357	279	0.04%	0.005%
31	5.923	1438	1441	1444	rVB	266	201	0.03%	0.003%
32	5.943	1444	1447	1450	rBV2	255	254	0.04%	0.004%
33	5.972	1450	1456	1458	rBV2	1302	1337	0.19%	0.022%
34	6.071	1482	1487	1490	rBV	254	287	0.04%	0.005%
35	6.242	1527	1540	1564	rBV	254940	498756	70.85%	8.230%
36	6.454	1602	1606	1608	rBV2	188	186	0.03%	0.003%

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Misc : 3.10g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0SK8ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Title : VOC Analysis

37	6.492	1612	1618	1619	rBV2	263	243	0.03%	0.004%
38	6.525	1619	1628	1640	rVB6	5800	10575	1.50%	0.174%
39	6.595	1640	1650	1656	rBV3	1659	2931	0.42%	0.048%
40	6.682	1664	1677	1698	rBV	162971	319221	45.34%	5.267%
41	6.817	1713	1719	1724	rVB4	483	577	0.08%	0.010%
42	6.972	1765	1767	1770	rBV2	268	199	0.03%	0.003%
43	7.197	1829	1837	1843	rBV4	2093	3560	0.51%	0.059%
44	7.496	1925	1930	1935	rBV2	269	362	0.05%	0.006%
45	7.560	1939	1950	1971	rVV	74340	136172	19.34%	2.247%
46	7.705	1987	1995	1998	rBV4	1309	1754	0.25%	0.029%
47	7.814	2025	2029	2032	rVB2	296	258	0.04%	0.004%
48	7.891	2041	2053	2072	rBV	304492	536186	76.16%	8.848%
49	8.049	2097	2102	2105	rBV2	344	327	0.05%	0.005%
50	8.078	2108	2111	2114	rVV2	302	211	0.03%	0.003%
51	8.177	2131	2142	2162	rVV	51184	91991	13.07%	1.518%
52	8.283	2172	2175	2179	rBV3	248	210	0.03%	0.003%
53	8.460	2226	2230	2238	rVB2	265	306	0.04%	0.005%
54	8.550	2248	2258	2269	rVB4	14087	23788	3.38%	0.393%
55	8.637	2274	2285	2315	rBV	188493	407165	57.84%	6.719%
56	8.804	2336	2337	2341	rBV	291	215	0.03%	0.004%
57	8.901	2364	2367	2369	rBV2	336	255	0.04%	0.004%
58	9.078	2420	2422	2428	rVB2	283	263	0.04%	0.004%
59	9.106	2428	2431	2433	rBV2	261	188	0.03%	0.003%
60	9.145	2436	2443	2446	rBV2	261	366	0.05%	0.006%
61	9.415	2514	2527	2545	rBV	378278	648988	92.19%	10.709%
62	9.569	2570	2575	2578	rBV2	970	1029	0.15%	0.017%
63	9.698	2607	2615	2628	rVB4	2810	4951	0.70%	0.082%
64	9.778	2634	2640	2643	rBV2	282	349	0.05%	0.006%
65	10.110	2735	2743	2748	rBV2	860	1358	0.19%	0.022%
66	10.261	2785	2790	2793	rBV2	282	237	0.03%	0.004%
67	10.287	2793	2798	2801	rBV	236	255	0.04%	0.004%
68	10.386	2826	2829	2834	rBV2	270	245	0.03%	0.004%
69	10.560	2877	2883	2888	rBV2	249	398	0.06%	0.007%
70	10.753	2931	2943	2962	rBV	269038	443499	63.00%	7.318%
71	10.891	2977	2986	2994	rBV2	1105	1733	0.25%	0.029%
72	11.036	3029	3031	3034	rVB	485	252	0.04%	0.004%
73	11.055	3034	3037	3042	rBV2	301	323	0.05%	0.005%
74	11.100	3045	3051	3055	rVV	417	488	0.07%	0.008%
75	11.328	3115	3122	3129	rVB2	1185	1460	0.21%	0.024%
76	11.450	3156	3160	3161	rBV	291	233	0.03%	0.004%

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 ALS Vial : 38 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0SK8ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
 Title : VOC Analysis

77	11.479	3161	3169	3178	rVB3	1075	1905	0.27%	0.031%
78	11.560	3189	3194	3197	rBV2	239	255	0.04%	0.004%
79	11.746	3249	3252	3255	rBV2	504	349	0.05%	0.006%
80	11.811	3259	3272	3293	rBV	407509	666550	94.68%	10.999%
81	12.190	3374	3390	3416	rBV	325293	542288	77.03%	8.948%
82	12.434	3460	3466	3470	rBV2	181	206	0.03%	0.003%
83	12.598	3512	3517	3519	rBV	188	215	0.03%	0.004%
84	12.769	3562	3570	3577	rVB2	1445	1865	0.26%	0.031%
85	13.058	3655	3660	3662	rBV2	273	257	0.04%	0.004%
86	13.161	3689	3692	3696	rVB2	380	253	0.04%	0.004%
87	13.293	3727	3733	3736	rVB2	362	419	0.06%	0.007%
88	13.312	3736	3739	3741	rBV	250	190	0.03%	0.003%
89	13.396	3759	3765	3767	rBV	230	253	0.04%	0.004%
90	13.563	3813	3817	3819	rBV	434	387	0.05%	0.006%
91	13.717	3858	3865	3868	rBV2	504	656	0.09%	0.011%
92	13.794	3883	3889	3892	rBV2	354	361	0.05%	0.006%
93	14.029	3958	3962	3964	rBV	299	240	0.03%	0.004%
94	14.090	3971	3981	4003	rBV	28384	54051	7.68%	0.892%
95	14.248	4027	4030	4036	rBV3	398	534	0.08%	0.009%
96	14.573	4123	4131	4139	rBV2	1349	2462	0.35%	0.041%
97	15.000	4261	4264	4273	rVB3	484	467	0.07%	0.008%
98	15.235	4330	4337	4347	rBV3	2997	5702	0.81%	0.094%
99	15.418	4388	4394	4400	rBV3	1650	2461	0.35%	0.041%
100	16.161	4622	4625	4626	rBV2	419	231	0.03%	0.004%

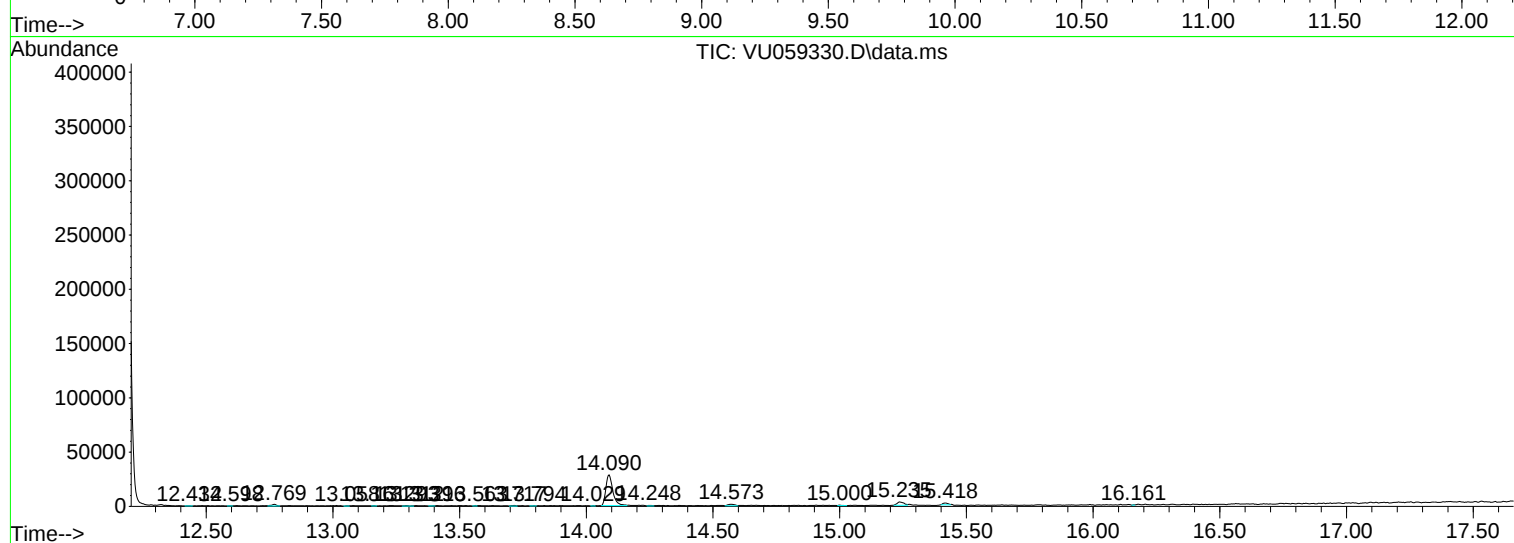
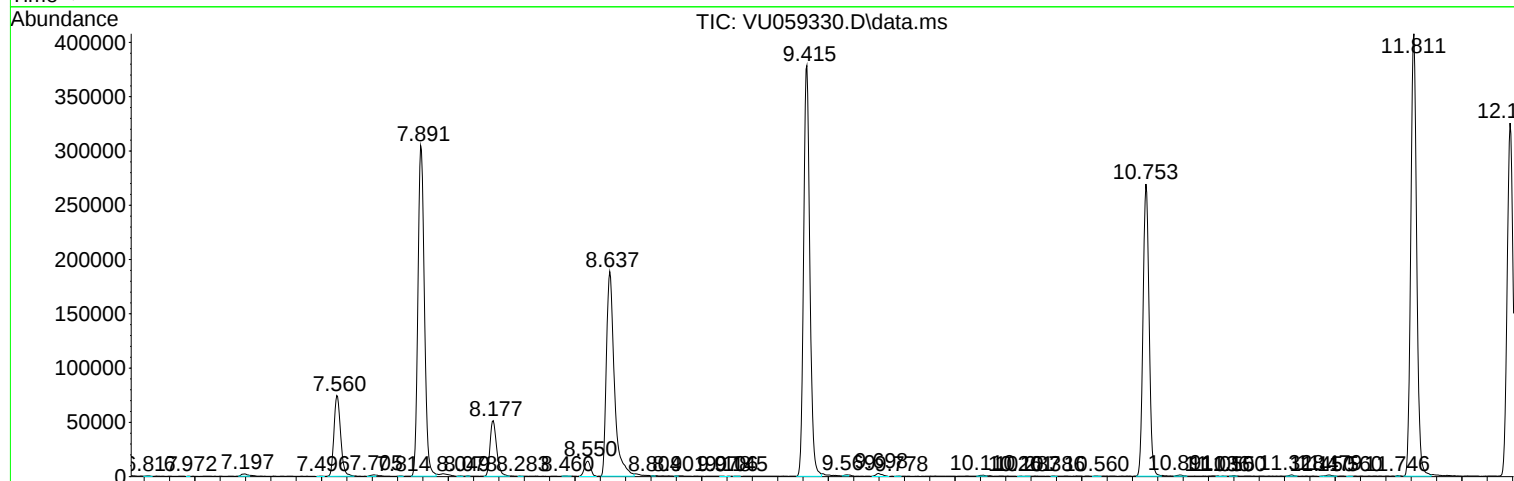
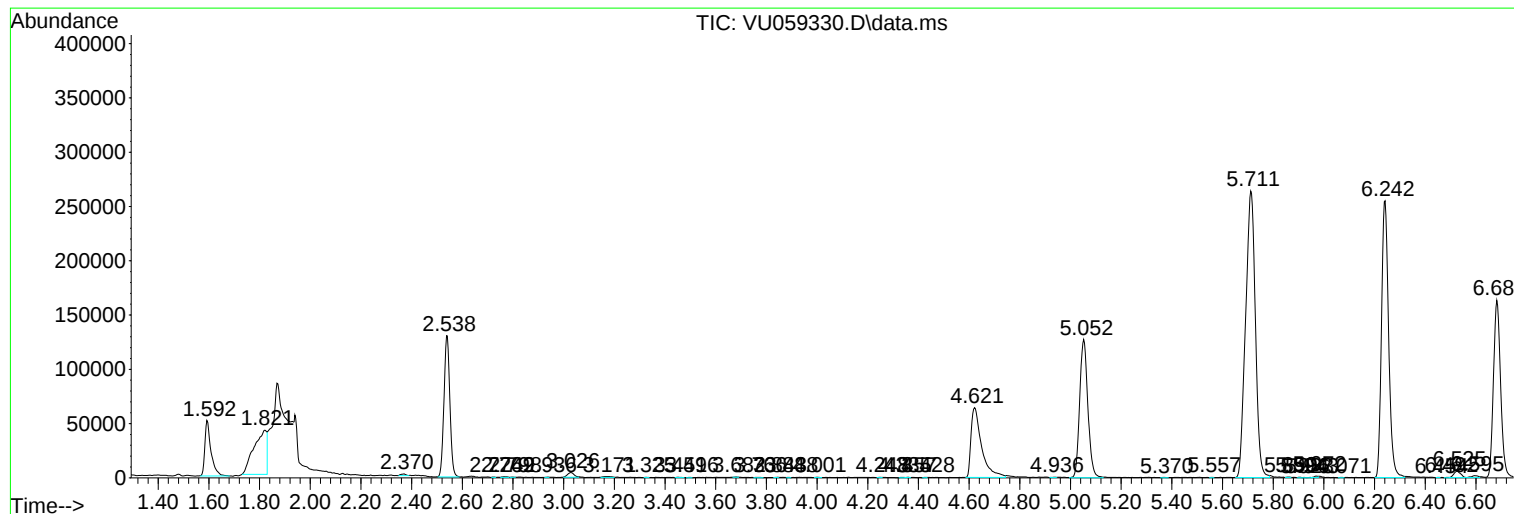
Sum of corrected areas: 6060296

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061824\
Data File : VU059330.D
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Sample : P2873-19ME
Misc : 3.10g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0SK8ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061824\
Data File : VU059330.D
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Operator : MD/SY
Sample : P2873-19ME
Misc : 3.10g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0SK8ME

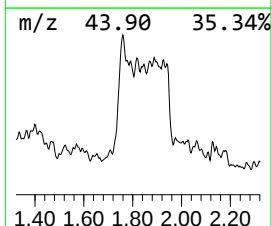
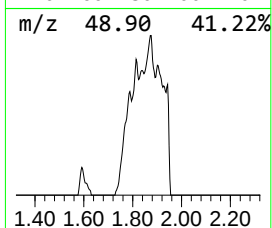
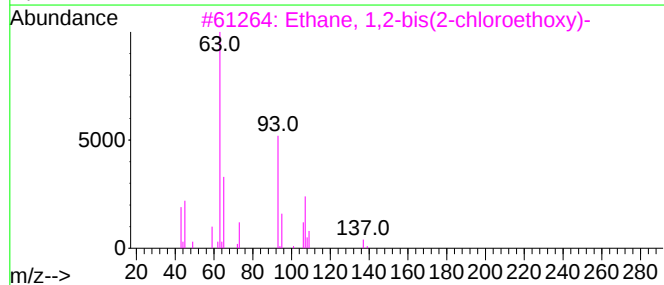
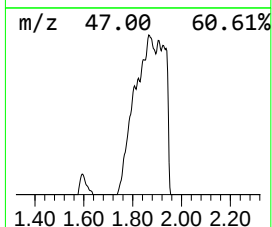
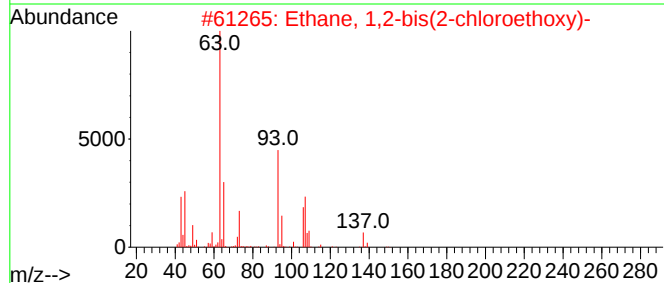
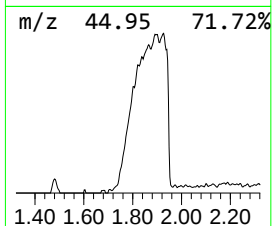
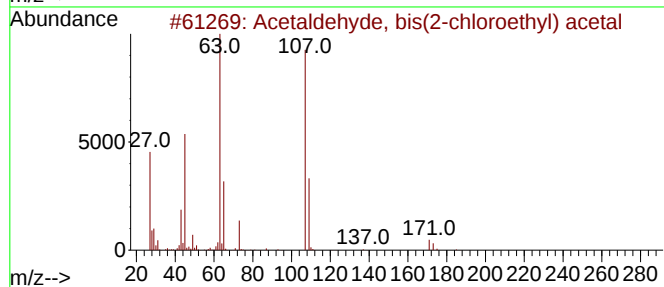
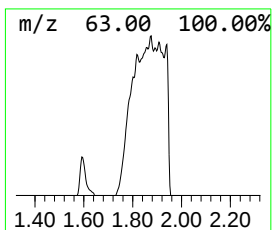
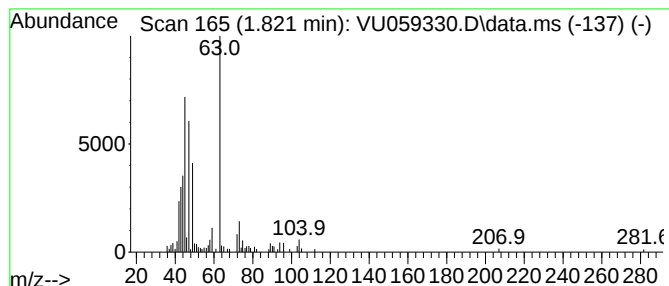
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.821	14.63 ug/L	145909	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde, bis(2-chloroethyl)...	186	C6H12Cl2O2	014689-97-5	28
2			Ethane, 1,2-bis(2-chloroethoxy)-	186	C6H12Cl2O2	000112-26-5	25
3			Ethane, 1,2-bis(2-chloroethoxy)-	186	C6H12Cl2O2	000112-26-5	9
4			.alpha.-Chloroethyl chloroformate	142	C3H4Cl2O2	050893-53-3	9
5			2-Chloropropionyl chloride	126	C3H4Cl2O	007623-09-8	9



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Operator : MD/SY
Sample : P2873-19ME
Misc : 3.10g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0SK8ME

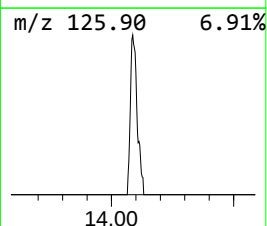
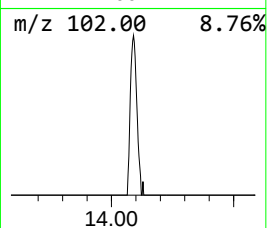
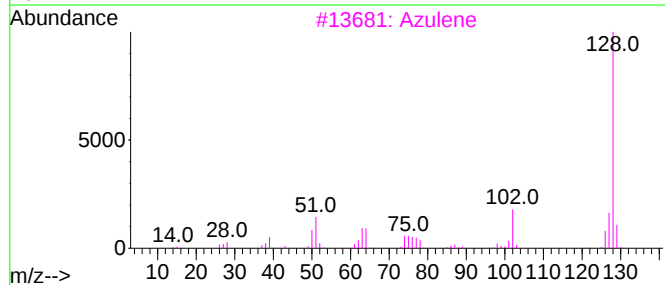
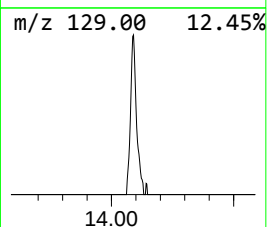
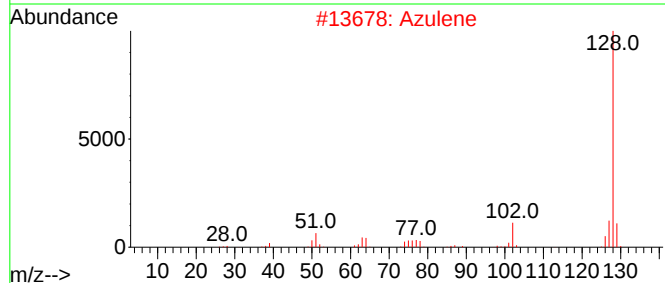
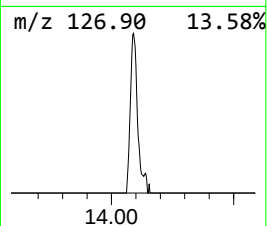
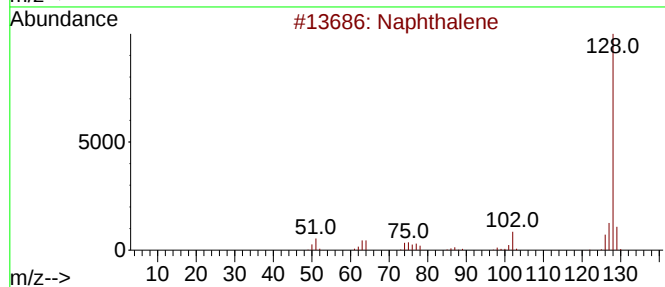
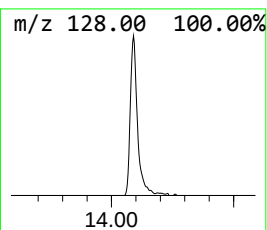
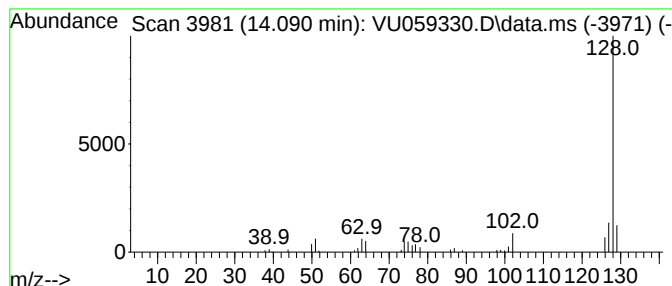
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Azulene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.090	4.05 ug/L	54051	1,4-Dichlorobenzene-d4	11.811

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			Azulene	128	C10H8	000275-51-4	93
3			Azulene	128	C10H8	000275-51-4	91
4			Azulene	128	C10H8	000275-51-4	91
5			Naphthalene	128	C10H8	000091-20-3	91



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Operator : MD/SY
Sample : P2873-19ME
Misc : 3.10g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0SK8ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.821	14.6	ug/L	145909	1	6.242	498756	50.0
Azulene	14.090	4.0	ug/L	54051	3	11.811	666550	50.0